LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
Data File : BM014203.D
Acq On : 08 Feb 2018 21:10
Operator : SJ/JU
Sample : J1469-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : WABUT-4

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.716	292	294	300	rVB2	35833	50325	1.15%	0.153%
2	5.163	364	370	386	rBV	1912299	2776418	63.25%	8.458%
3	6.734	630	637	651	rBV	2032828	3140578	71.55%	9.567%
4	7.075	689	695	711	rBV	2051704	3202364	72.96%	9.755%
5	7.539	768	774	783	rBV	405595	646482	14.73%	1.969%
6	7.851	820	827	838	rBV	1489809	2406939	54.84%	7.332%
7	8.698	963	971	985	rBV	1112011	1989120	45.32%	6.059%
8	10.310	1239	1245	1259	rBV	409628	809967	18.45%	2.467%
9	12.804	1662	1669	1682	rBV	2603835	3929692	89.53%	11.971%
10	13.668	1810	1816	1831	rBV2	119724	255504	5.82%	0.778%
11	14.098	1884	1889	1897	rBV2	57790	86410	1.97%	0.263%
12	14.198	1899	1906	1914	rBV2	662270	1044605	23.80%	3.182%
13	15.057	2047	2052	2057	rVB	71730	91175	2.08%	0.278%
14	15.698	2152	2161	2174	rBV	1931823	2953002	67.28%	8.996%
15	15.927	2195	2200	2210	rBV3	62006	123843	2.82%	0.377%
16	16.956	2369	2375	2385	rBV	729258	1159676	26.42%	3.533%
17	17.739	2502	2508	2514	rBV5	27652	57803	1.32%	0.176%
18	17.862	2522	2529	2539	rBV2	170035	281383	6.41%	0.857%
19	19.033	2719	2728	2733	rBV9	21572	58819	1.34%	0.179%
20	19.150	2744	2748	2755	rBV8	43338	75447	1.72%	0.230%
21	19.597	2818	2824	2832	rBV	3756961	4389365	100.00%	13.371%
22	20.874	3038	3041	3048	rBV4	104782	161552	3.68%	0.492%
23	21.162	3085	3090	3100	rBV	912738	1249106	28.46%	3.805%
24	22.309	3280	3285	3291	rVB	427657	551608	12.57%	1.680%
25	23.338	3454	3460	3468	rVB	612743	1173918	26.74%	3.576%
26	25.309	3790	3795	3802	rVB9	69884	162386	3.70%	0.495%

Sum of corrected areas: 32827487

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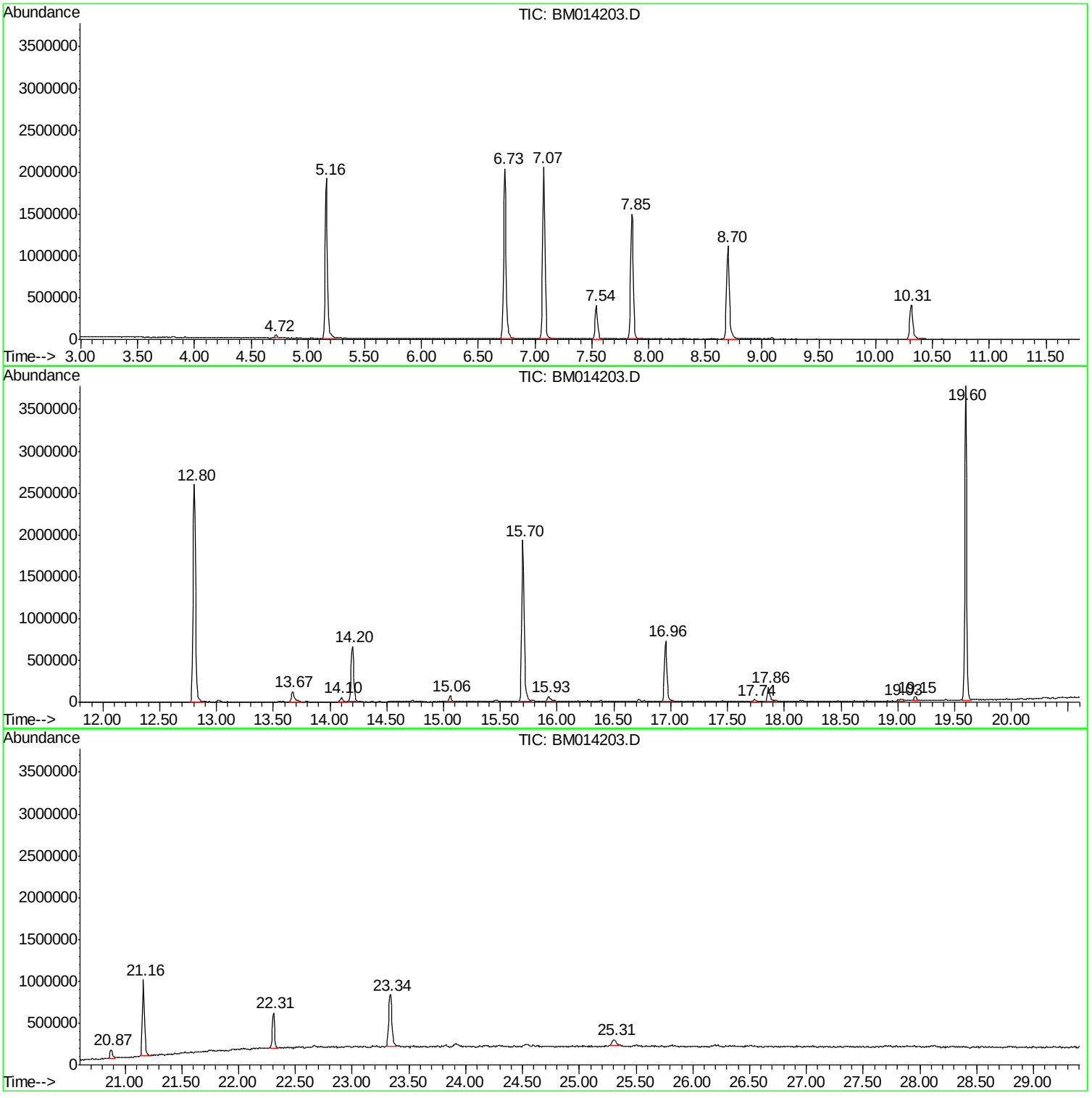
WABUT-4

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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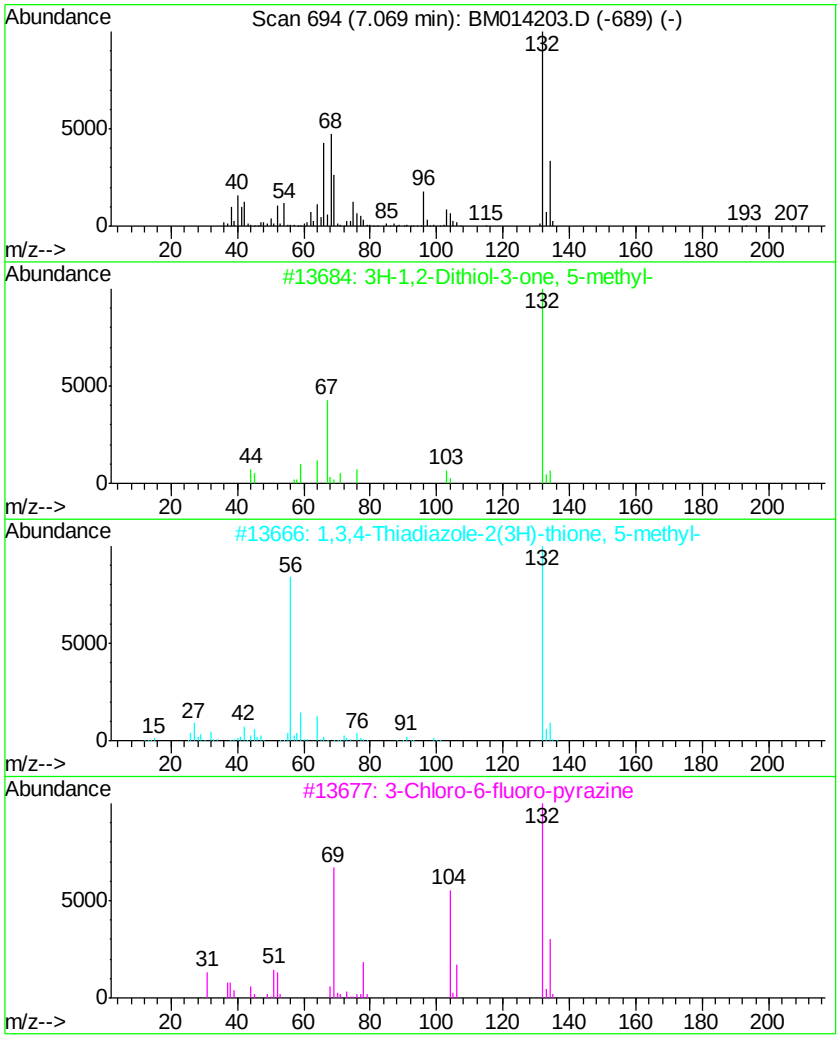
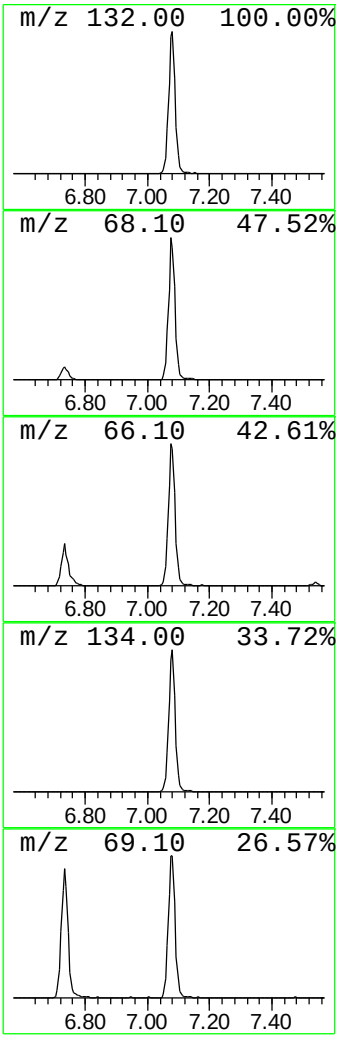
Peak Number 1 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	99.07 ng	3202360	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
2	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





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ClientSampleId : WABUT-4

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TIC Library : C:\DATABASE\NIST02.L
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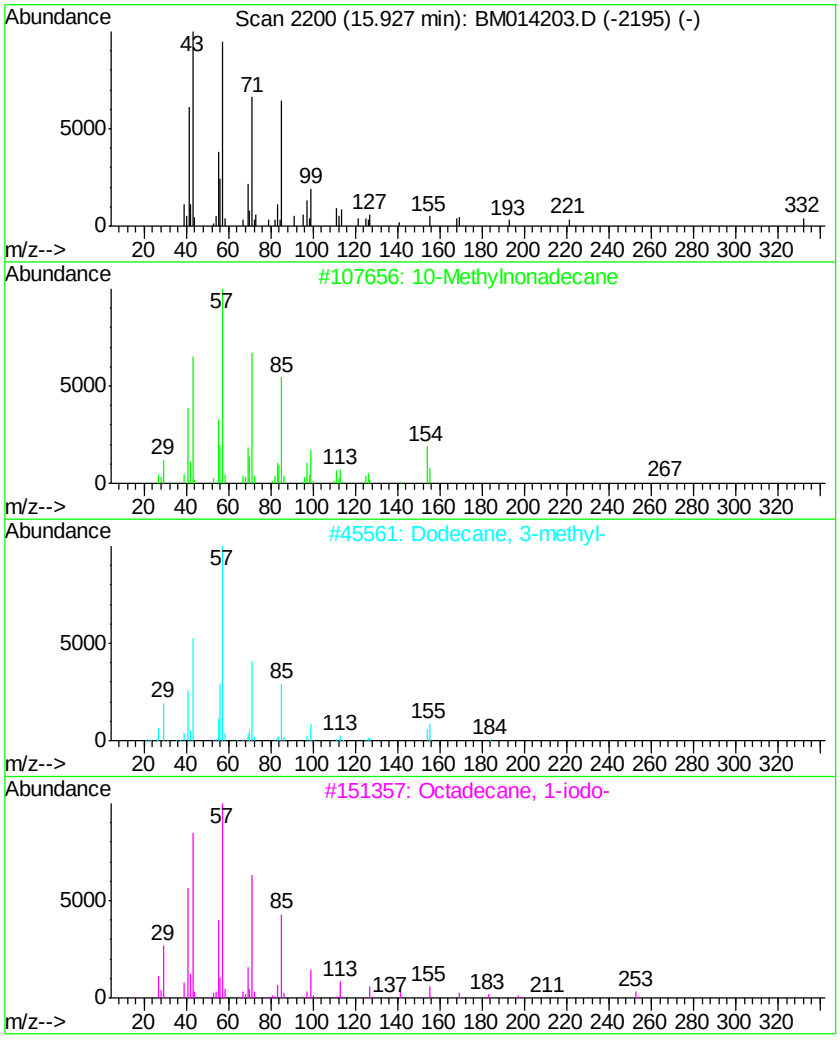
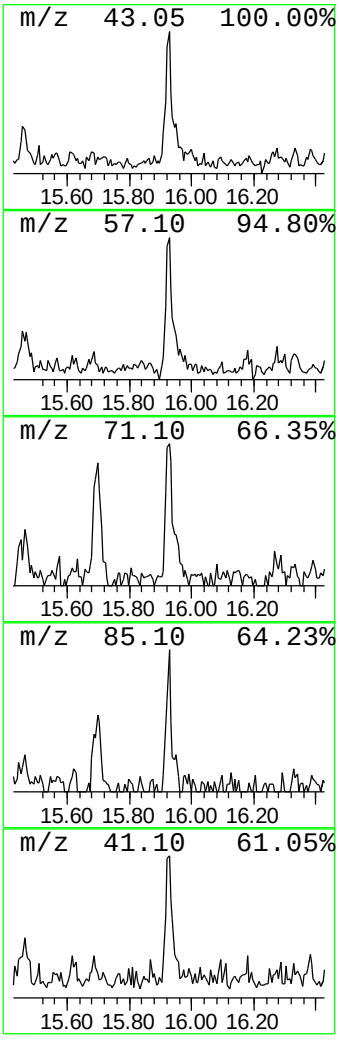
Peak Number 3 10-Methylnonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.14 ng	123843	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	86
2	Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
5	Nonadecane	268	C19H40	000629-92-5	64





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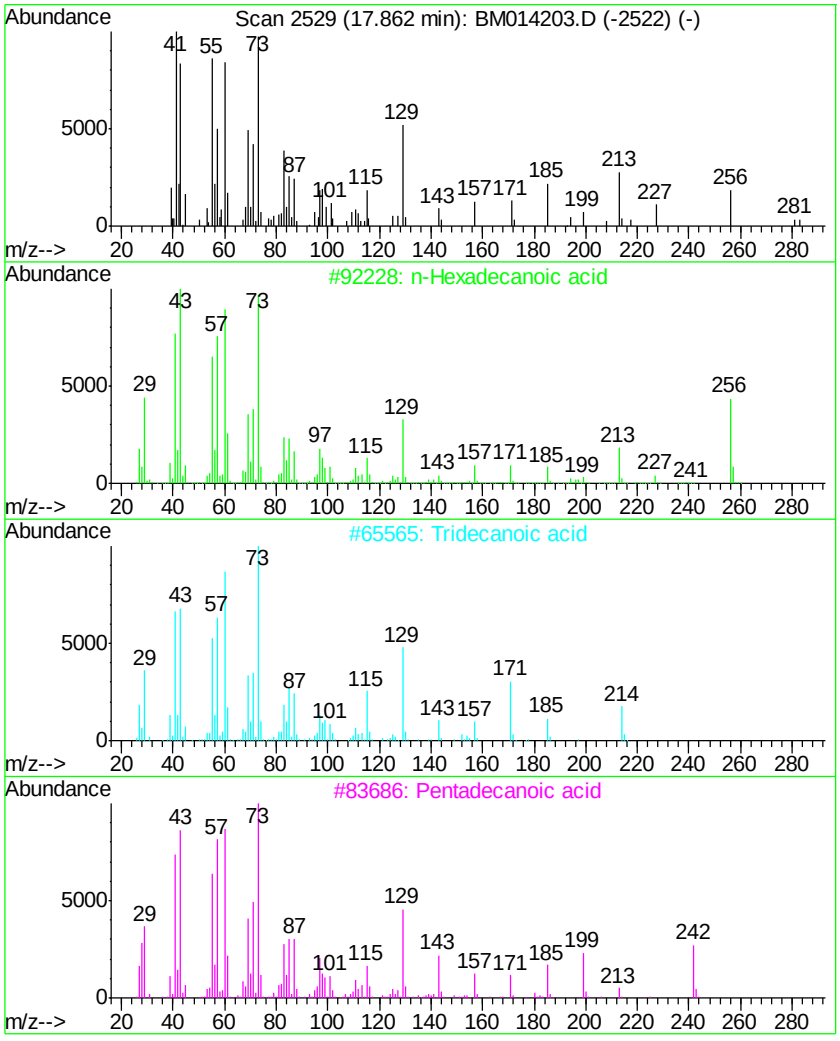
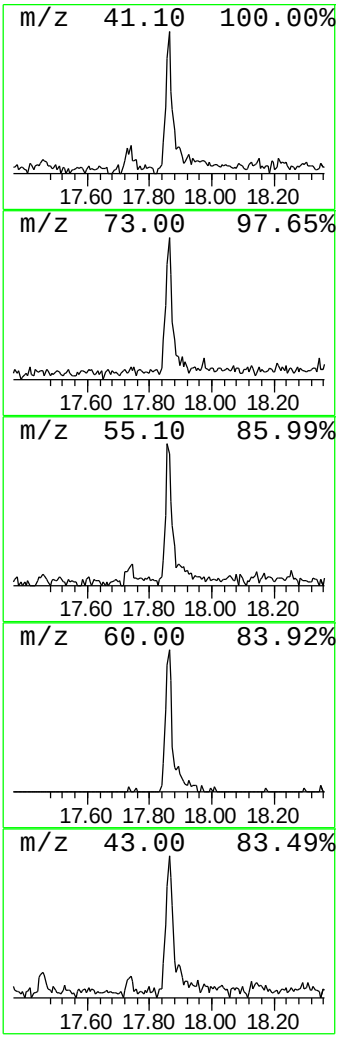
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	4.85 ng	281383	Phenanthrene-d10	16.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Tridecanoic acid	214	C13H26O2	000638-53-9	68
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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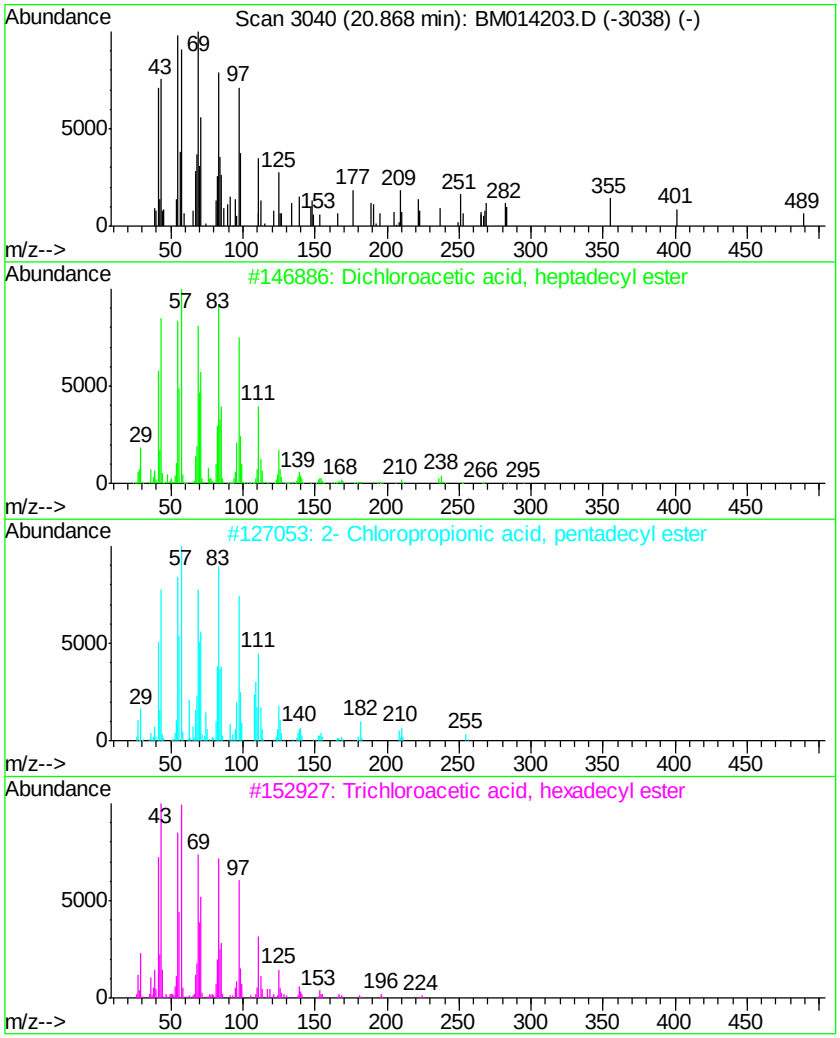
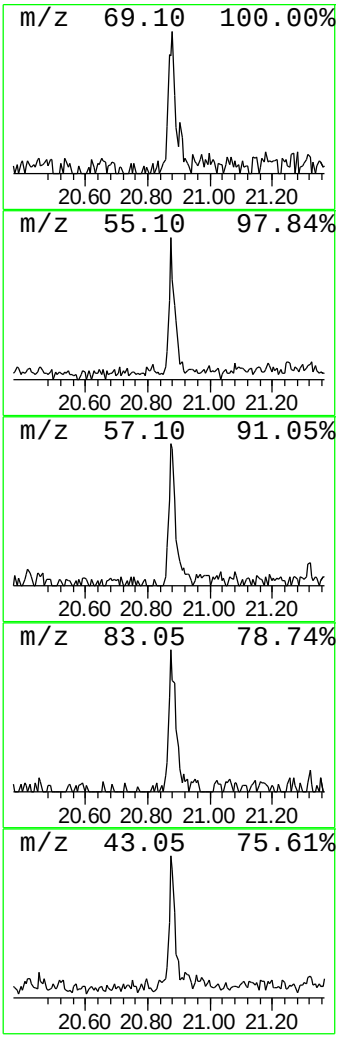
Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	2.59 ng	161552	Chrysene-d12	21.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87





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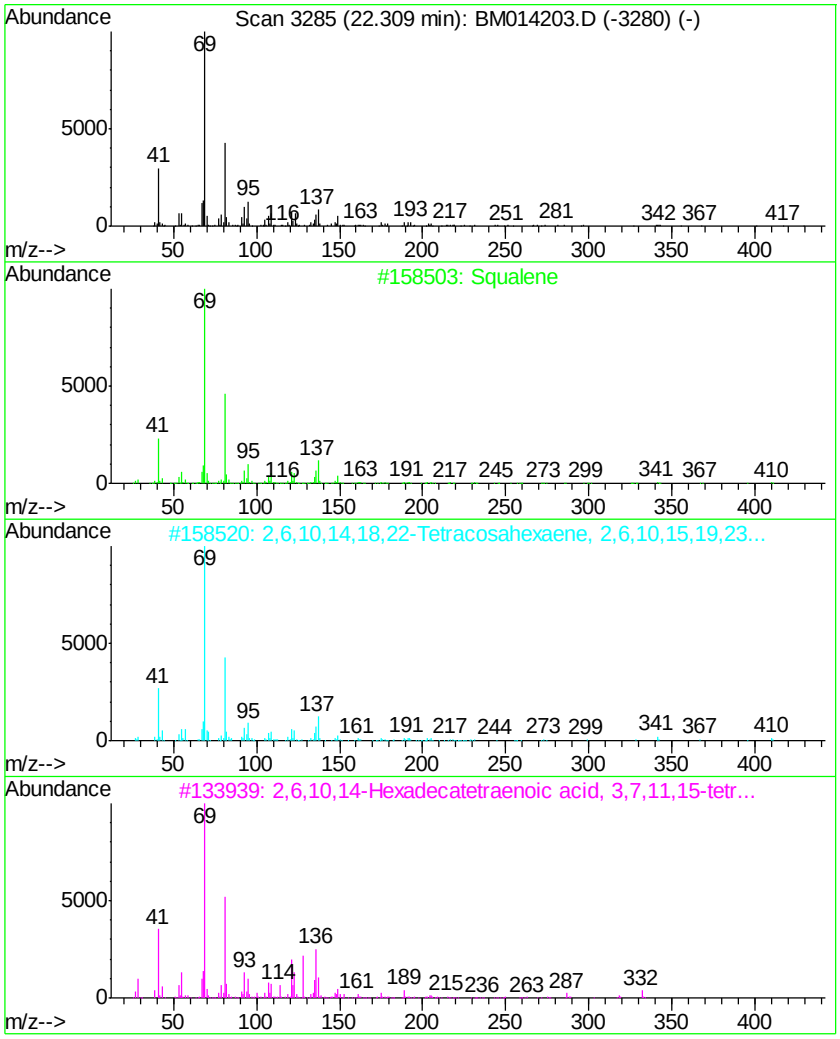
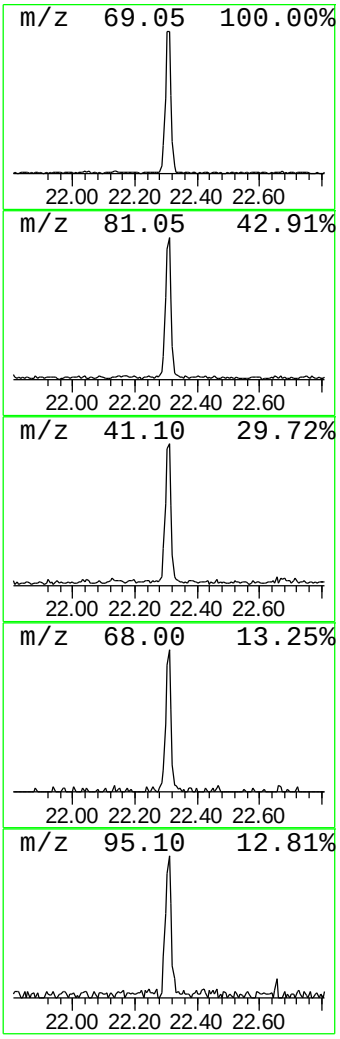
Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.31	9.40 ng	551608	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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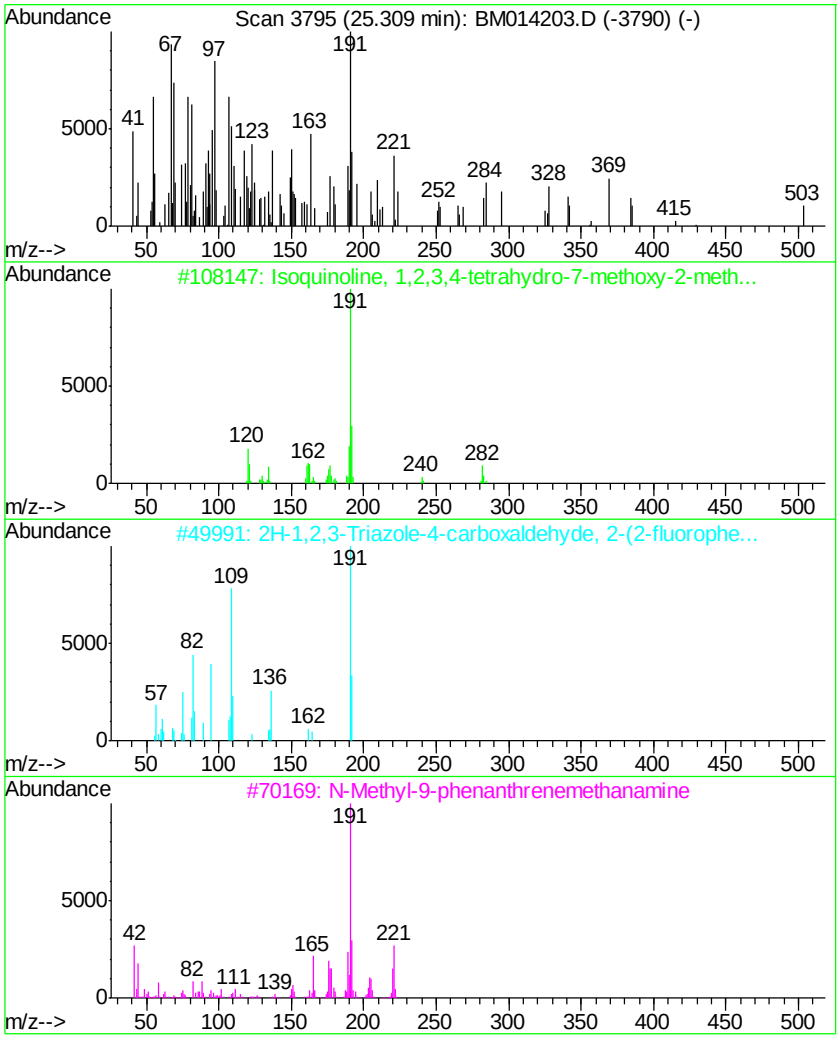
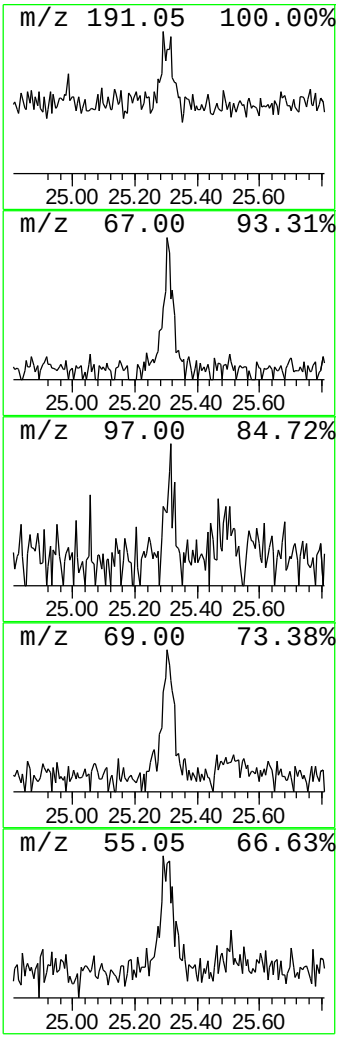
Peak Number 7 unknown25.31 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.31	2.77 ng	162386	Perylene-d12	23.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	27
2	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	18
3	N-Methyl-9-phenanthrenemethanamine	221	C16H15N	076532-36-0	14
4	Benzene, 1-butyl-4-(diethoxymeth...	236	C15H24O2	083803-80-9	14
5	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	14





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown7.07	7.07	99.1	ng	3202360	1	7.54	646482	20.0
10-Methylnonadecane	15.93	2.1	ng	123843	4	16.96	1159680	20.0
n-Hexadecanoic acid	17.86	4.8	ng	281383	4	16.96	1159680	20.0
Dichloroacetic ac...	20.87	2.6	ng	161552	5	21.16	1249110	20.0
Squalene	22.31	9.4	ng	551608	6	23.34	1173920	20.0
unknown25.31	25.31	2.8	ng	162386	6	23.34	1173920	20.0